

Distribution Function of Electron Velocity Perpendicular to the Driving Force in a Uniform Nonequilibrium Steady State

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A macroscopically uniform model of a two-dimensional electron system is proposed to study nonequilibrium properties of electrical conduction. By molecular dynamics simulation, the steady state distribution function P_y of electron velocity in a direction perpendicular to an external driving force is calculated. An explicit form of P_y is determined within the accuracy of the numerical simulation, which fits the numerical data well even in the regime where a local equilibrium description is not valid. Although the entire structure of P_y is different from that of a local equilibrium distribution function, the asymptotic structure of the tails of P_y in the limit of large absolute values of the velocity is identical to that of a Maxwell distribution function with a temperature which is different from that in the equilibrium state and the kinetic temperature in the steady state.

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One of the central roles of statistical mechanics is to provide a principle for calculating the probability distribution ρ of a microscopic state without solving equations of motion. In equilibrium states it is given as the canonical distribution. In nonequilibrium steady states (NESSs), by contrast, such a principle is not known.

In studies of nonequilibrium systems with some concrete models, it is generally easier to compute a single-particle distribution function, such as a velocity distribution function (VDF), than to calculate ρ itself. In equilibrium states, the VDF is, of course, the Maxwell distribution. Although the VDF contains less information than ρ since the VDF is a marginal probability distribution, it yields a restriction on ρ and knowledge of the VDF is thus expected to provide a clue to finding a principle of nonequilibrium statistical mechanics.

VDFs have been investigated mainly in models described by kinetic equations, such as the Boltzmann equation and the Bhatnagar-Gross-Krook equation [1]. Such kinetic models are said to be valid for dilute gas systems. Furthermore, VDFs in most studies on those models are given as a power series of degrees of nonequilibrium (such as a temperature gradient). From these facts, it may be interesting to investigate a model other than kinetic models using a method without power series expansions.

One of the approaches in such studies is molecular dynamics (MD) simulation on models which obey microscopic equations of motion. VDFs have been investigated with MD simulations in shear-flowing systems [2] and thermal-conducting lattice systems [3, 4]. In those studies, deviations from local equilibrium distribution functions (LEDs) have mainly been considered. However, sufficient characterization of VDFs from the viewpoint of statistical mechanics has not yet been achieved. Another example of MD simulations was a study of the dis-

tribution function of energy currents carried by a single particle in thermal-conducting particle systems [5]. In that work, the authors found that the energy current distribution function has tails at large absolute values of the current, which are well described by equilibrium distributions with appropriate temperatures. This tail structure might be a universal property of steady state distribution functions. That is, for a wide range of nonequilibrium systems, including thermal-conducting and other systems, tails of distributions such as VDFs and energy current distributions might asymptotically approach certain equilibrium distributions, although the complete structures would be different from those of the equilibrium distributions.

In the present paper, to demonstrate the above idea, we investigate a VDF in an electrically conducting system. We introduce a model in which a macroscopically uniform NESS is realized, and perform MD simulation to calculate a VDF in a direction perpendicular to an external driving force. We find an explicit form of the VDF within simulation accuracy. Introduction of a velocity-dependent “reciprocal temperature” helps to determine the form.

Model. The system of the simulation is composed of electrons, phonons, and impurities, which are modeled as classical particles. A schematic diagram of the system is shown in the inset of Fig. 1. The linear dimension in the α -direction of the system is denoted by L_α ($\alpha = x, y, z$). Electrons (whose mass, charge, and total number are denoted by m_e , e , and N_e) can move only in a two-dimensional (2D) x - y plane (shown in dark gray) which is located on the top ($z = L_z$) of the three-dimensional (3D) system. Phonons (whose mass and total number are denoted by m_p and N_p) can move throughout the entire 3D system. Impurities (whose total number is denoted by N_i) are fixed at random positions, and play the role of a random potential. N_i^{2D} of the impurities are uniformly distributed throughout the 2D electron system and N_i^{3D} throughout the 3D system under the 2D system ($N_i^{2D} + N_i^{3D} = N_i$). Periodic boundary

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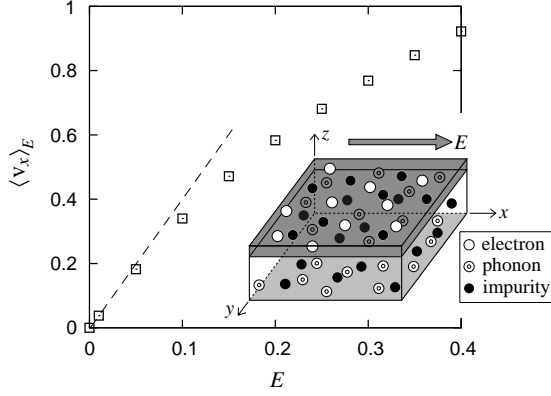


FIG. 1: Average of electron velocity in the x -direction, plotted against E . The dashed line represents the slope of the linear response. Inset: schematic diagram of the simulation system. Electrons are confined in a 2D plane (dark gray). Under the 2D electron system there is a three-dimensional phonon system, the bottom of which is a thermal wall (light gray). Impurities are distributed throughout all regions of the system. An external electric field E is applied in the x -direction.

conditions are imposed in the x - and y -directions. The boundary conditions in the z -direction, applied only to phonons, are an elastic potential wall for the top boundary ($z = L_z$) and a thermal wall (shown in light gray) with temperature T_0 for the bottom boundary ($z = 0$). We apply an external electric field E (acting on electrons) uniformly in the x -direction to drive the system to a nonequilibrium state. We assume that interactions among all kinds of particles are present. The interaction potential between the k -th and l -th particles is given by $\phi_{kl} = \mathcal{V}(\max\{0, d_{kl}\})^{5/2}$. Here, \mathcal{V} is a constant of interaction strength, and $d_{kl} = R_k + R_l - r_{kl}$ is the overlap of the potential ranges. R_k is the radius of the potential range (R_e , R_p , and R_i for an electron, phonon, and impurity, respectively), and r_{kl} is the inter-center distance between the particles. The energy supplied from E to electrons is transferred to phonons by electron-phonon interactions and dissipates through the thermal walls, by which the system retains its energy balance. In the simulations we take e , R_e , m_e , a reference energy, and the Boltzmann constant as the units, and fix the following parameters: $L_x = L_y = 200$, $L_z = 10$, $R_p = R_i = 1$, $m_p = 1$, $T_0 = 1$, $N_e = 1000$, $N_p = 4000$, $N_i^{2D} = 500$, $N_i^{3D} = 1000$, and $\mathcal{V} = 4000$.

This model is an extension of the two-dimensional model for the MD simulation of electrical conduction, which has been previously proposed in Ref. [6]. A possible experimental situation corresponding to the model in Ref. [6] occurs when the edges of a 2D electron system are in contact with large sample holders (which have large heat capacity and good heat conduction). On the other hand, the present model is a reflection of a typical experimental setup of a quasi-2D electron system in

a semiconductor device. That is, a 2D electron system is realized around the top of a bulk substrate (which is modeled by the 3D system of phonons and impurities) and the substrate is mounted on a large sample holder (which is modeled by the thermal wall). The present model is macroscopically uniform in the y -direction as well as in the x -direction, whereas the previous one was uniform only in the direction parallel to E . This enables us to investigate bulk properties in both the x - and y -directions. It should also be noted that this model is isotropic in the y -direction and the net currents of particles and energy in this direction are absent on average.

In Fig. 1 we show E -dependence of the average electron velocity $\langle v_x \rangle_E$ in the x -direction. Here $\langle \cdots \rangle_E$ denotes the average in the steady state for E . A linear response is observed in the regime of small E and a nonlinear response in the regime of large E .

Deviation from LEDF. Because of the macroscopic spatial uniformity of the model, steady states in the model are also uniform. That is, local quantities such as local number densities and local kinetic temperatures in steady states are almost independent of the position in the 2D electron plane. We may therefore use electrons in the entire region of the plane to calculate a VDF of electrons. In this paper we investigate distribution functions $P_y(v_y)$ of electron velocity v_y in the y -direction. [The corresponding results in the x -direction (parallel to E) will be presented elsewhere [7]; these have more complicated structures and properties than those of P_y presented here.] In Fig. 2 we show semi-logarithmic plots of P_y , plotted against v_y^2 . The data for positive v_y almost completely overlap with those for negative v_y in NESSs ($E = 0.1$ and 0.4), as well as in the equilibrium state ($E = 0$). This indicates that $P_y(v_y)$ is symmetric at $v_y = 0$, and is consistent with $\langle v_y \rangle_E = 0$, even in the nonlinear response regime. These results are due to the isotropy in the y -direction of the model.

As an LEDF in the y -direction, we employ a naive distribution function defined by

$$f_y^{\text{loc}}(v_y) = \sqrt{m_e/2\pi T_e^y} \exp(-m_e v_y^2/2T_e^y), \quad (1)$$

where $T_e^y = m_e \langle v_y^2 \rangle_E$ is a kinetic temperature in this direction (this is simply a Maxwell distribution with temperature T_e^y). In Fig. 2 we also plot f_y^{loc} (in this plot zero-mean Gaussian distributions are drawn as straight lines). We observe that the tails of P_y and f_y^{loc} are different for large values of E , whereas they are almost the same for $E = 0$. Moreover in the inset of Fig. 2, we plot the deviation $P_y(v_y) - f_y^{\text{loc}}(v_y)$. From this figure we see that the difference around $v_y = 0$ is also large in the NESSs. The symmetric behavior of the deviation is again consistent with the isotropic nature of the model.

Explicit form of P_y . To explore the functional form of P_y we next investigate a v_y -dependent “reciprocal temperature”, $\beta_y(v_y)$, which is defined by

$$\beta_y(v_y) = -\frac{2 \ln [P_y(v_y)/P_y(0)]}{m_e v_y^2}. \quad (2)$$

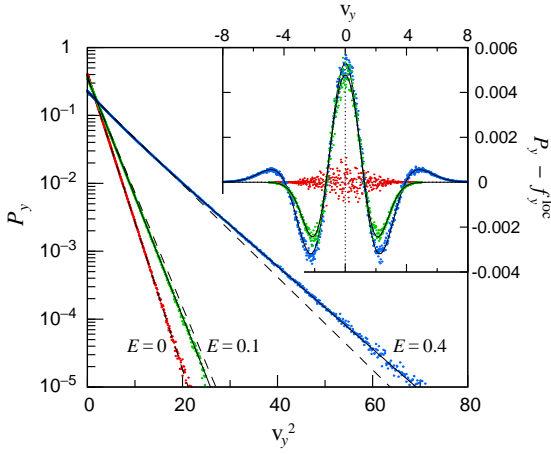


FIG. 2: (Color online) A semi-logarithmic plot of the distribution P_y , plotted against v_y^2 . The results for $E = 0, 0.1$, and 0.4 are shown. The data for $v_y > 0$ and $v_y < 0$ are overlapped. The dashed lines represent the LEDFs f_y^{loc} . The solid lines depict fitting curves of Eq. (4) for $E = 0.1$ and 0.4 . Inset: deviation $P_y(v_y) - f_y^{\text{loc}}(v_y)$ from the LEDF. Also shown are the fitting curves of Eq. (4), with f_y^{loc} subtracted, for $E = 0.1$ and 0.4 (solid curves).

If P_y is a Maxwell distribution, β_y is independent of v_y and is equal to the reciprocal temperature of the Maxwell distribution. In Fig. 3 we show v_y -dependence of β_y . Figure 3 (a) is a result for the equilibrium state ($E = 0$). In this case β_y is almost independent of v_y and is nearly equal to the reciprocal temperature $1/T_0$ ($= 1$) of the thermal wall within the precision of the numerical simulation. This is consistent with the fact that in an equilibrium state, P_y is a Maxwell distribution with T_0 . Although the data fluctuations are rather large for v_y 's close to zero and in the tails, they are simply due to the restricted accuracy of the numerical simulation in these regions and they can be expected to become smaller as we average over greater numbers of simulation samples.

Figures 3 (b) and (c) show the results for NESSs ($E = 0.1$ and 0.4 , respectively). As $|v_y|$ becomes large, β_y varies (increasing in (b) and decreasing in (c)) monotonically and tends to converge to a certain constant value β_y^∞ , which is different from both $1/T_0$ and $1/T_e^y$. This implies that P_y approaches a Maxwell distribution as $|v_y| \rightarrow \infty$. Furthermore, we find that the overall behavior of β_y is well described by a Gaussian function. That is, β_y is well fitted by

$$\beta_y(v_y) = B \exp(-Dv_y^2) + \beta_y^\infty, \quad (3)$$

where β_y^∞ , B , and D are fitting parameters. In the insets of Figs. 3 (b) and (c), to see this more clearly, we show semi-logarithmic plots of $|\beta_y - \beta_y^\infty|$ versus v_y^2 . We observe exponential decay behavior of $|\beta_y - \beta_y^\infty|$ as functions of v_y^2 , which indicates that the variation of $|\beta_y - \beta_y^\infty|$ is almost equivalent to that of Gaussian functions of v_y . Although the data for v_y 's close to zero and in the tails

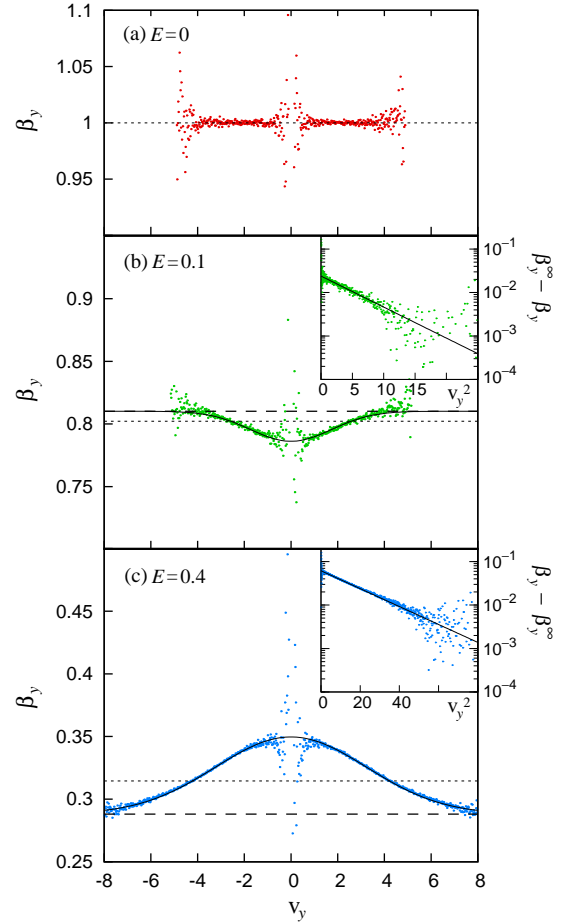


FIG. 3: (Color online) Mains: β_y for (a) $E = 0$, (b) $E = 0.1$, and (c) $E = 0.4$, plotted against v_y . The dotted and dashed lines represent $1/T_e^y$ and β_y^∞ , respectively ($1/T_e^y \simeq \beta_y^\infty \simeq 1/T_0 = 1$ when $E = 0$). The solid lines are fitting curves of Eq. (3). Insets: semi-logarithmic plots of (b) $\beta_y^\infty - \beta_y$ and (c) $\beta_y - \beta_y^\infty$, respectively, plotted against v_y^2 . The data for $v_y > 0$ and $v_y < 0$ are overlapped. The solid straight lines represent fitting curves of Eq. (3) (subtracted from β_y^∞ in (b) and reduced by β_y^∞ in (c), respectively).

fluctuate rather violently, they would converge to a single curve as the number of samples increases. From Eqs. (2) and (3) we thus obtain an explicit functional form of P_y as

$$P_y(v_y) = P_y(0) \exp \left[- \left(\beta_y^\infty + B e^{-Dv_y^2} \right) \frac{m_e v_y^2}{2} \right]. \quad (4)$$

This is a main result of the present paper. In Fig. 2 we plot curves of Eq. (4) for $E = 0.1$ and 0.4 as solid lines. These also reveal that Eq. (4) is a good fitting function of P_y for almost all values of v_y .

E-dependence. Figure 4 shows the E -dependences of parameters in Eq. (4). In the top of Fig. 4 we compare β_y^∞ and $1/T_e^y$. Although E -dependences of these two quantities are similar, their detailed values are different. $\beta_y^\infty > 1/T_e^y$ at small values of E (as can be seen also

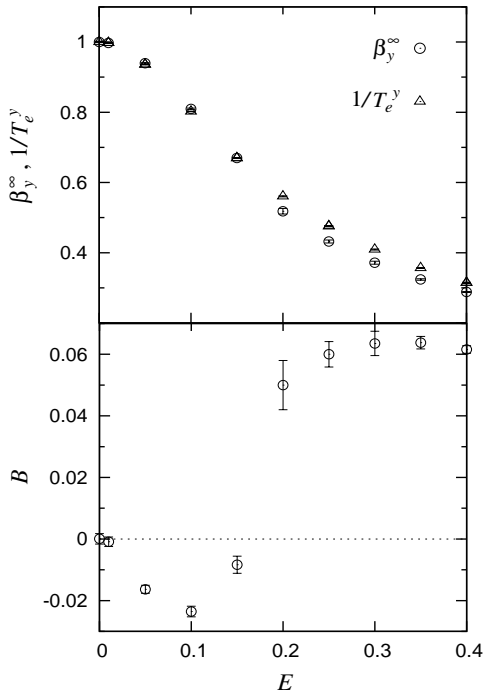


FIG. 4: Top: E -dependence of β_y^∞ (circles) and $1/T_e^y$ (triangles). Bottom: E -dependence of B .

in Fig. 3 (b)), whereas $\beta_y^\infty < 1/T_e^y$ at large values of E (as is seen also in Fig. 3 (c)). In the bottom of Fig. 4 we show the result for B . There exists a value E_c of the electric field such that $B < 0$ if $0 < E < E_c$ and $B > 0$ if $E > E_c$ ($E_c \simeq 0.15$ in the parameter values of the present simulation). This is consistent with the result for β_y^∞ , which is mentioned above. That is, $\beta_y^\infty > 1/T_e^y$ if $0 < E < E_c$ and $\beta_y^\infty < 1/T_e^y$ if $E > E_c$.

Summary and discussion. In this paper we have introduced a model of a two dimensional classical electron system which is macroscopically uniform. In the model with an external driving force (electric field E), a spatially uniform nonequilibrium steady state (NESS) is realized. By using molecular dynamics simulations we have investigated the distribution function $P_y(v_y)$ of an electron velocity v_y in a direction perpendicular to E in a steady state. When the driving force is large, the local equilibrium (LE) description is not valid. We have determined an explicit form of the velocity distribution func-

tion (VDF) as Eq. (4), which is valid up to numerical accuracy, even for NESSs where the LE description breaks down. The functional form has a velocity-dependent “reciprocal temperature” $\beta_y(v_y)$. In the limit of large absolute values of v_y , this reciprocal temperature converges to a constant value β_y^∞ , which is different from both the equilibrium temperature and the kinetic temperature, and the VDF thus approaches asymptotically a Maxwell distribution with temperature $1/\beta_y^\infty$. We have also found that there exists a crossing value of the driving force below (above) which $\beta_y^\infty > \beta_y(0)$ ($\beta_y^\infty < \beta_y(0)$). It might be difficult to obtain such a nontrivial dependence of β_y on E by a naive perturbation expansion in terms of E .

The asymptotic property of the tails of the VDFs in NESSs is similar to that of nonequilibrium distribution functions of microscopic energy currents in thermal conduction models [5]. In those models the distribution function of energy currents parallel to the temperature gradient has a tail for large negative (positive) values of the current which asymptotically obeys an equilibrium distribution with temperature T_- (T_+). Here, T_- and T_+ are different from the local temperature at the place where the distribution is measured, but equal to the local kinetic temperatures at slightly forward and backward regions, respectively. In the present model of electrical conduction, the tails of the VDF asymptotically obey an equilibrium distribution with temperature $1/\beta_y^\infty$. Although $1/\beta_y^\infty$ is equivalent in the tails for positive and negative values of velocity (because of the isotropy of the model in the direction perpendicular to the driving force), it differs from both the equilibrium temperature and the kinetic temperature. We therefore expect that it is a universal feature in NESSs that the distribution function of a microscopic current approaches an equilibrium distribution in the limit of large currents. This might be related to a representation of the nonequilibrium distribution of microscopic states, which has been derived recently [8].

Unlike the results for thermal conduction models, we do not yet know the physical meaning of the temperature $1/\beta_y^\infty$. Also we do not understand the meanings of other parameters in the functional form of the VDF and the crossing value of the driving force. These subjects remain for future research.

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